Theses and Dissertations   1. Thesis and Dissertation Collection, all items

1972

Acoustic energy flow in high symmetry crystals.

Fauth, Herbert Carl.

http://hdl.handle.net/10945/15967

ACOUSTIC ENERYG FLOW IN
HIGH SYMMETRY CRYSTALS

Herbert Carl Fauth

NAVAL POSTGRADUATE SCHOOL
Monterey, California
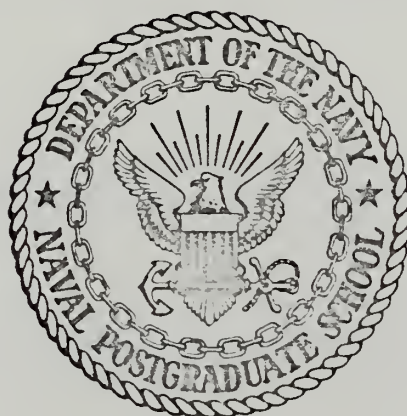
THESIS

ACOUSTIC ENERGY FLOW

IN

HIGH SYMMETRY CRYSTALS

by

Herbert Carl Fauth

Thesis Advisor: J. R. Neighbours

June 1972

Acoustic Energy Flow in High Symmetry Crystals

by

Herbert Carl Fauth
Lieutenant, United States Navy
B.S., United States Naval Academy, 1967

Submitted in partial fulfillment of the
requirements for the degree of

MASTER OF SCIENCE IN PHYSICS

from the

NAVAL POSTGRADUATE SCHOOL
June 1972

ABSTRACT

The determination of elastic properties of crystals by sound velocity measurements is facilitated by use of a perturbation solution to the equations of motion for sound waves propagating in the crystals. Transformation equations can relate the solution for arbitrary porpagation direction to an established crystal coordinate system. A method of calculating the acoustic components of the energy flow vector is developed for several high symmetry crystal classes. The validity of this method is herein confirmed and results are presented which are consistent with experimental data. A modern desk calculator was employed to determine solutions for hexagonal, cubic and tetragonal crystals.

TABLE OF CONTENTS

A major portion of the theoretical development presented in this paper has previously been presented by Prof. John R. Neighbours, Physics Department, U. S. Naval Postgraduate School. The most recent paper, co-authored by Associate Professor G. E. Schacher, Physics Department, U. S. Naval Postgraduate School, is titled "Determination of Elastic Constants from Sound Velocity Measurements in Crystals of General Symmetry." In addition, several investigators have published methods similar to this development. These papers are included in the List of References.

I. INTRODUCTION

The task of relating velocity measurements to elastic constants of a crystal is complicated by the fact that the eigenvectors which describe the direction of vibration in response to the sound wave are neither perpendicular nor parallel to the propagation direction. The energy flow may, however, be described by modes of vibration which are quasi-longitudinal (essentially parallel to the propagation direction). In practice one vibrational mode dominates the others for a given propagation direction. In addition the transducer used to measure the velocity has greater response to one mode of vibration so it is possible to separate modes by appropriate choice of transducers.

For certain high symmetry crystal classes special directions of propagation exist in which the response is pure longitudinal and pure transverse. Velocity measurements along these directions can be directly related to crystal elastic constants. However the energy flow is not necessarily parallel to the propagation.

For either high or low symmetry cases the elastic constants can be determined by solution of the crystal vibration equation of motion. This process may be simplified by appropriate choice of coordinate system and application of several assumptions. The resultant secular equation is solved by a perturbation method and the values for the elastic constants may be refined by iteration. The constants thus obtained are

linear combinations of the elastic constants defined by conventional coordinate systems and can be converted by rotational transformation. The angle of deviation of the energy flow vector from the propagation direction is of particular interest in order to construct a physical picture of the crystal response. This angle can be obtained by application of the general energy flow equations to the coordinate system defined by the propagation direction.

II. SECULAR EQUATION

The general form of Hooke's Law is

$$T_{ij} = C_{ijkl}S_{kl} \tag{1}$$

Two common conventions of subscript notation for the above equation are shown below.
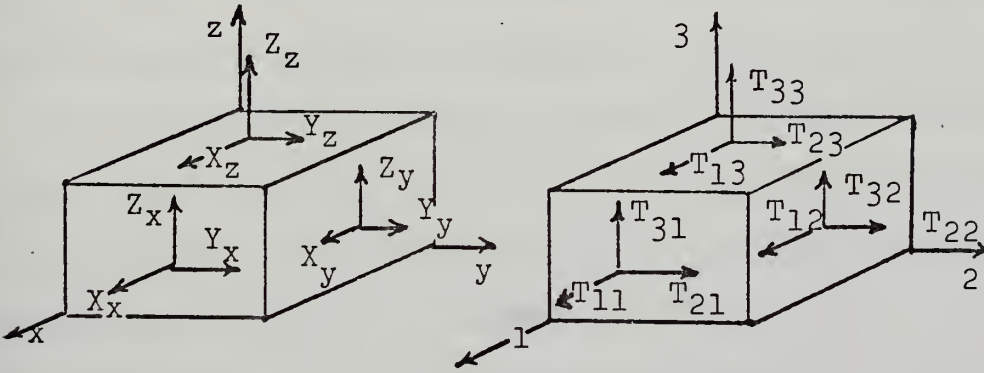

FIGURE 1

The strain, S, is related to displacement by the equation

$$S_{kl} = \frac{1}{2}(u_{k,l} + u_{l,k}) = \frac{1}{2}\left(\frac{\partial u_k}{\partial u_l} + \frac{\partial u_l}{\partial u_k}\right) \tag{2}$$

where u is displacment. In contracted notation Hooke's Law may be written as

$$T_i = C_{ij}S_j \tag{3}$$

where the following notation applied:

$$X_x = T_{11} = T_1$$

$$Y_y = T_{22} = T_2$$

$$Z_z = T_{33} = T_3$$

$$Y_z = Z_y = T_{23} = T_{32} = T_4 \qquad (4)$$

$$X_z = Z_x = T_{13} = T_{31} = T_5$$

$$X_y = Y_x = T_{12} = T_{21} = T_6$$

The existence of a strain energy function reduces the 36 elastic constants to 21 independent constants for the most general case. This number can be further reduced for specific crystal calsses because of symmetry considerations.

If an arbitrary coordinate system is chosen such that the x' axis lies along the direction of propagation the equations of motion can be written in terms of the elastic constants in the arbitrary coordinate system and displacement. In this development u', v', w' are displacements along the x', y', and z' axes respectively. The primed notation emphasizes the fact that choice of coordinate system is arbitrary. The equations of motion are

$$F_{x'} = ma = \rho \, \frac{\partial^2 u'}{\partial t^2} \, dx'dy'dz' = \rho \left(\frac{\partial T_1}{\partial x'} + \frac{\partial T_6}{\partial y'} + \frac{\partial T_5}{\partial z'} \right) dx'dy'dz'$$

$$\frac{\partial^2 u'}{\partial t^2} = \frac{\partial}{\partial x'} \left(C'_{11}S'_1 + C'_{12}S'_2 + C'_{13}S'_3 + C'_{14}S'_4 + C'_{15}S'_5 + C'_{16}S'_6 \right.$$

$$\left. + \frac{\partial T_6}{\partial y'} + \frac{\partial T_5}{\partial z'} \right. \qquad (5)$$

If plane wave propagation is assumed the partial derivatives with respect to y' and z' vanish and the equation becomes

$$F_{x'} = C'_{11} \frac{\partial^2 u'}{\partial x'^2} + C'_{16} \frac{\partial^2 v'}{\partial x'^2} + C'_{15} \frac{\partial^2 w'}{\partial x'^2} \qquad (6)$$

Similarly, the equations of motion for the remaining directions are

$$F_{y'} = \rho \frac{\partial^2 v'}{\partial t^2} = C'_{16} \frac{\partial^2 u'}{\partial x'^2} + C'_{66} \frac{\partial^2 v'}{\partial x'^2} + C'_{56} \frac{\partial^2 w'}{\partial x'^2}$$

$$F_{z'} = \rho \frac{\partial^2 w'}{\partial t^2} = C'_{15} \frac{\partial^2 u'}{\partial x'^2} + C'_{56} \frac{\partial^2 v'}{\partial x'^2} + C'_{55} \frac{\partial^2 w'}{\partial x'^2}$$

An additional assumption is that the solutions are periodic of the form

$$u' = A_1 \cos(kx' - \omega t)$$

$$v' = A_2 \cos(kx' - \omega t) \qquad (7)$$

$$w' = A_3 \cos(kx' - \omega t)$$

The assumed periodic solutions are inserted in the equations of motion and the partial derivatives are evaluated. The resultant equations may be further simplified by the relation $V = \omega/k$ where V represents velocity and is not to be confused with v', the displacement in the y' direction. The equations may now be written

$$\begin{bmatrix} A_1(C'_{11} - V^2) & A_2C'_{16} & A_3C'_{15} \\ A_1C'_{16} & A_2(C'_{66} - V^2) & A_3C'_{56} \\ A_1C'_{15} & A_2C'_{56} & A_3(C'_{55} - V^2) \end{bmatrix} \begin{bmatrix} u' \\ v' \\ w' \end{bmatrix} = 0 \quad (8)$$

The secular equation has three real roots corresponding to
one quasi-longitudinal and two transverse modes of vibration.
If the solutions are assumed to be essentially longitudinal
or transverse with small deviations from these directions
the secular equation yields a perturbation solution:

$$C'_{11} = \rho V_1^2 - \frac{1}{A_1}\left[\frac{A_1 A_3 C'^2_{15}}{A_3(C'_{11} - C'_{55})} + \frac{A_1 A_2 C'^2_{16}}{A_2(C'_{11} - C'_{66})} + \ldots \ldots \right]$$

Note that the amplitudes of the assumed periodic solutions do
not affect the calculation. The remaining solutions to the
perturbation equations are

$$C'_{66} = \rho V_2^2 - \left[\frac{C'^2_{16}}{C'_{66} - C'_{11}} + \frac{C'^2_{56}}{C'_{66} - C'_{55}} + \ldots \ldots \right]$$

$$C'_{55} = \rho V_3^2 - \left[\frac{C'^2_{15}}{C'_{55} - C'_{11}} + \frac{C'^2_{56}}{C'_{55} - C'_{66}} + \ldots \ldots \right] \quad (9)$$

In particular, if the terms in square brackets vanish the
solutions correspond to pure mode response and the elastic
constants are determined directly from the measured velocities.
When the square bracketed terms are present velocity measure-
ments along several directions yield an adequate number of
equations to determine all six elastic constants of the secular

equation to first order. These values are then inserted in
the square bracketed terms and the solution is refined. The
primed elastic constants are linear combinations of those
defined by the conventional coordinate system. The rotational
transformation relating the two systems is developed in
Section IV.

The amplitudes of the periodic solutions may be determined
from the equations of motion. If the amplitude of one mode
of interest is fixed at an arbitrary value the remaining two
amplitudes can be expressed in terms of the elastic constants
and the measured velocities. For example, if the amplitude
A_1 is set equal to unity the longitudinal mode solution is

$$
A_2 = \frac{\left[\dfrac{\rho V_1^2 - c_{11}''}{c_{15}'} - \dfrac{c_{15}'}{\rho V_3^2 - c_{55}'}\right]}{\left[\dfrac{c_{16}'}{c_{15}'} + \dfrac{c_{56}'}{\rho V_3^2 - c_{55}'}\right]}
$$

$$
A_3 = \frac{\left[\dfrac{\rho V_1^2 - c_{11}'}{c_{16}'} + \dfrac{c_{15}'}{c_{56}'}\right]}{\left[\dfrac{\rho V_3^2 - c_{55}'}{c_{56}'} + \dfrac{c_{15}'}{c_{16}'}\right]}
$$

(10)

III. ENERGY FLOW

The components of the Energy Flow vector are[1]

$$E_{x'} = \dot{u}'X_x' + \dot{v}'X_y' + \dot{w}'X_z'$$

$$E_{y'} = \dot{u}'Y_x' + \dot{v}'Y_y' + \dot{w}'Y_z' \tag{11}$$

$$E_{z'} = \dot{u}'Z_x' + \dot{v}'Z_y' + \dot{w}'Z_z'$$

The x' component of this vector can be calculated as follows:

$$E_{x'} = \dot{u}' \left(C_{11}' \frac{\partial u'}{\partial x'} + C_{16}' \frac{\partial v'}{\partial x'} + C_{15}' \frac{\partial w'}{\partial x'} \right)$$

$$+ \dot{v}' \left(C_{16}' \frac{\partial u'}{\partial x'} + C_{66}' \frac{\partial v'}{\partial x'} + C_{56}' \frac{\partial w'}{\partial x'} \right) \tag{12}$$

$$+ \dot{w}' \left(C_{15}' \frac{\partial u'}{\partial x'} + C_{56}' \frac{\partial v'}{\partial x'} + C_{55}' \frac{\partial w'}{\partial x'} \right)$$

Note that the plane wave assumption has been applied to yield only those terms which contain partial derivatives with respect to x'. The transverse components of the Energy Flow vector are

$$E_{y'} = \dot{u}' \left(C_{16}' \frac{\partial u'}{\partial x'} + C_{66}' \frac{\partial v'}{\partial x'} + C_{56}' \frac{\partial w'}{\partial x'} \right)$$

$$+ \dot{v}' \left(C_{12}' \frac{\partial u'}{\partial x'} + C_{26}' \frac{\partial v'}{\partial x'} + C_{25}' \frac{\partial w'}{\partial x'} \right) \tag{13}$$

$$+ \dot{w}' \left(C_{14}' \frac{\partial u'}{\partial x'} + C_{46}' \frac{\partial v'}{\partial x'} + C_{45}' \frac{\partial w'}{\partial x'} \right)$$

---

[1] A. E. H. Love, A Treatise on the Mathematical Theory of Elasticity (New York, 1944), ch. 7.

$$E_{z'} = \dot{u}' \left(C_{15}' \frac{\partial u'}{\partial x'} + C_{66}' \frac{\partial v''}{\partial x'} + C_{55}' \frac{\partial w''}{\partial x'} \right)$$

$$+ \dot{v}' \left(C_{14}' \frac{\partial u'}{\partial x'} + C_{46}' \frac{\partial v''}{\partial x'} + C_{45}' \frac{\partial w''}{\partial x'} \right)$$

$$+ \dot{w}' \left(C_{13}' \frac{\partial u'}{\partial x'} + C_{36}' \frac{\partial v''}{\partial x'} + C_{35}' \frac{\partial w''}{\partial x'} \right)$$

On substitution of the periodic solutions the x' component becomes

$$E_{x'} = \omega A_1 \sin \eta \, [C_{11}'(-kA_1 \sin \eta) + C_{16}'(-kA_2 \sin \eta)$$

$$+ C_{15}'(-kA_3 \sin \eta)] + \omega A_2 \sin \eta \, [C_{16}'(-kA_1 \sin \eta)$$

$$+ C_{66}'(-kA_2 \sin \eta) + C_{56}'(-kA_3 \sin \eta)]$$

$$+ \omega A_3 \sin \eta \, [\ldots]$$

where $\eta = kx' - \omega t$.

The above form may be further simplified by defining

$$P_{x'} \equiv \frac{E_{x'}}{-\omega k \sin^2 \eta}$$

The final form of the Energy Flow components is shown below.

$$P_{x'} = C_{11}' A_1^2 + C_{66}' A_2^2 + C_{55}' A_3^2 + 2C_{16}' A_1 A_2 + 2C_{15}' A_1 A_3 + 2C_{56}' A_2 A_3$$

$$P_{y'} = C_{16}' A_1^2 + C_{26}' A_2^2 + C_{45}' A_3^2 + (C_{66}' + C_{12}') A_1 A_2 + (C_{56}' + C_{14}') A_1 A_3$$

$$(C_{25}' + C_{46}') A_2 A_3$$

13

$$P_{z'} = C'_{15}A_1^2 + C'_{46}A_2^2 + C'_{35}A_3^2 + (C'_{56} + C'_{14})A_1A_2 + (C'_{55} + C'_{13})A_1A_3$$

$$(C'_{45} + C'_{36})A_2A_3 \qquad\qquad (15)$$

The resultant Energy Flow vector determines deviation from direction of propagation as shown in the diagram below. Note that the angle δ is the compliment of the polarization angle.
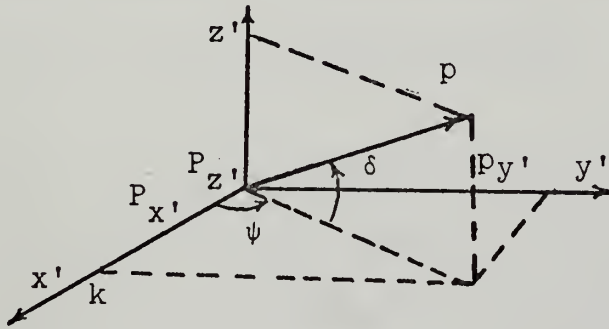
FIGURE 2

IV. TRANSFORMATION OF ELASTIC CONSTANTS

The desired elastic constants are defined by a fixed, unprimed coordinate system which is related to the crystal basis vectors a, b, c in accordance with convention adopted by the I.R.E. standards committee.[2] Specific examples of this convention are provided in Sections V, VI and VII. The primed coordinate system is chosen so that the x' axis lies in the x-y plane. This leads to a relationship between the two systems in terms of the direction cosines

$$\ell = \sin \theta \cos \phi$$
$$m = \sin \theta \sin \phi \qquad\qquad (16)$$
$$n = \cos \theta$$

FIGURE 3

---

[2] Standard Committee, "Standards on Piezoelectric Crystals," Proc. I.R.E. 37 (September, 1949), p. 1378.

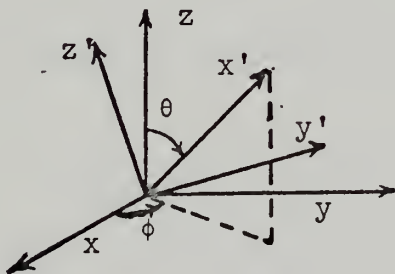The transformation elements are given in tabular form below.

	x	y	z
x'	ℓ	m	n
y'	$-m\alpha^{-1}$	$\ell\alpha^{-1}$	0
z'	$-\ell n\alpha^{-1}$	$-mn\alpha^{-1}$	α

$$\text{(17)}$$

The elements have been reduced by use of the definition $\alpha^2 \equiv \ell^2 + m^2$.

For example:

$$x = \ell x' - m\alpha^{-1}y' - \ell n\alpha^{-1}z' \qquad (18)$$

The transformation of elastic constants may be obtained from Hooke's Law;

$$T_i = C_{ij}S_j \qquad (19)$$

If the transformations of stress and strain are $T' = \beta T_i$ and $S' = \gamma S_i$ the elastic constants are related by the expression

$$C'_{ij} = \beta C_{ij}\gamma^{-1} \qquad (20)$$

where $\gamma^{-1} = \bar{\beta}$ and β is the matrix shown below.

$$
\begin{vmatrix}
\ell^2 & m^2 & n^2 & 2mn & 2\ell n & 2\ell m \\
m^2\alpha^{-2} & \ell^2\alpha^{-2} & 0 & 0 & 0 & -2\ell m\alpha^{-2} \\
\ell^2 n^2\alpha^{-2} & m^2 n^2\alpha^{-2} & \alpha^2 & -2mn & -2\ell n & \ell mn^2\alpha^{-2} \\
\ell mn\alpha^{-2} & -\ell mn\alpha^{-2} & 0 & \ell & -m & -n(\ell^2-m^2)\alpha^{-2} \\
-\ell^2 n\alpha^{-1} & -m^2 n\alpha^{-1} & n\alpha & m(1-2n^2)\alpha^{-1} & \ell(1-2n^2)^{-1} & -2\ell mn\alpha^{-1} \\
-\ell m\alpha^{-1} & \ell m\alpha^{-1} & 0 & \ell n\alpha^{-1} & -mn\alpha^{-1} & (\ell^2-m^2)\alpha^{-1}
\end{vmatrix}
$$

The Energy Flow equations and the rotational transformation may now be applied to specific crystal classes.

V. CRYSTALS OF HEXAGONAL SYMMETRY

In application to certain high symmetry crystal classes
the method is simplified due to symmetry considerations and
the fact that certain primed elastic constants may vanish.
This leads to a partially diagonal secular equation and the
existence of semi-pure modes of vibration. For hexagonal
crystals the I.R.E. convention defines the unprimed coordinate
system such that the z-axis is parallel to the crystal basis
vector c, i.e. the sixfold symmetry axis, and the x-axis is
parallel to a, the two fold rotation axis. The y-axis is
perpendicular to x and z to preserve a right handed coordinate
system. With this definition the primed elastic constants
become

$$C'_{11} = \alpha^4 C_{11} + 2n^2\alpha^2(C_{13} + 2C_{44}) + n^4 C_{33}$$

$$C'_{55} = n^2\alpha^2 C_{11} - n^2\alpha^2(2C_{13} - C_{33}) + (1-2n^2)^2 C_{44}$$

$$C'_{66} = \frac{1}{2}\alpha^2(C_{11} - C_{12}) + n^2 C_{44} \tag{22}$$

$$C'_{15} = -n\alpha^3 C_{11} + n\alpha(1-2n^2)(C_{13} + 2C_{44}) + n^3\alpha C_{33}$$

$$C'_{16} = C'_{56} = 0$$

Since C'_{16} and C'_{56} are zero the existence of a semi-pure mode
is implied. Physically this means that the vibrational response
of the crystal lies along one of the primed system axes for

17

one mode (pure transverse) and the remaining modes are quasi-longitudinal and quasi-transverse. The relative orientation of the eigenvector components to the propagation is shown below.
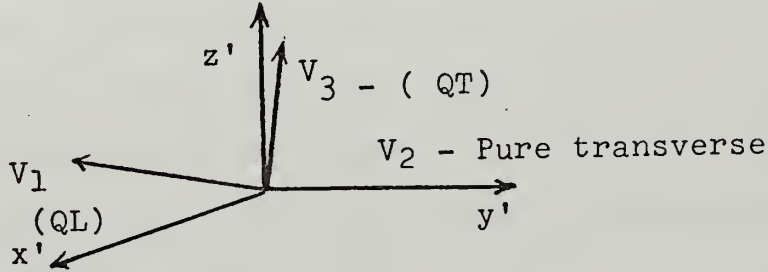

FIGURE 4

Note that if C_{15}' were to vanish the secular equation would become diagonal and the response would be pure longitudinal or transverse. This situation may occur for materials possessing hexagonal symmetry. The existence of this accidental pure mode was predicted by Borgnis[3] for the case of propagation in a direction that makes an angle θ with the c axis defined by

$$\tan^2 \theta = \frac{C_{33} - C_{13} - 2C_{44}}{C_{11} - C_{13} - 2C_{44}} \qquad (23)$$

The above requirement corresponds to the fact that C_{15}' vanishes and the secular equation is diagonal in the perturbation solution.

Equations (22) are sufficient to calculate the velocities of each of the modes from known values of conventional elastic

[3]F. E. Borgnis, "Specific Directions of Longitudinal Wave Propagation in Anisotropic Media," Phys. Rev. 98 (August, 1955), p. 1000.

constants. The elastic constants of numerous hexagonal crystals have already been determined and the application of the perturbation method may be demonstrated by comparison of calculated mode velocities with measured values. The solution for energy flow, however, requires nine additional constants i.e. C'_{12}, C'_{13}, C'_{14}, C'_{25}, C'_{26}, C'_{35}, C'_{36}, C'_{45}, C'_{46}. Some of these may vanish as a result of symmetry. For hexagonal symmetry C'_{14}, C'_{26}, C''_{36} and C''_{45} are all identically zero. The remaining primed constants are

$$C'_{12} = \alpha^2 C_{12} + n^2 C_{13}$$

$$C'_{13} = (1 - 2n^2\alpha^2)C_{13} + n^2\alpha^2(C_{11} + C_{33} - 4C_{44})$$

$$C'_{25} = n\alpha(C_{13} - C_{12}) \tag{24}$$

$$C'_{35} = -n\alpha(n^2 C_{11} + (1-2n^2)C_{13} - \alpha^2 C_{33} + 2(1-2n^2)C_{44})$$

$$C'_{46} = -\frac{1}{2}n\alpha(C_{11} - C_{12} - 2C_{44})$$

In addition, the fact that C''_{56} and C''_{16} are zero leads to simplified forms of the amplitude equations. With these simplifications the equations for energy flow in hexagonal crystals are

$$P_{x'} = C'_{11}A_1^2 + C'_{66}A_2^2 + C'_{55}A_3^2 + 2C'_{15}A_1A_3$$

$$P_{y'} = (C'_{66} + C'_{12})A_1A_2 + (C'_{25} + C'_{46})A_2A_3 \tag{25}$$

$$P_{z'} = C'_{15}A_1^2 + C'_{35}A_3^2 + (C'_{55} + C'_{13})A_1A_3 + C'_{46}A_2^2$$

Some of the terms in the above equations will vanish when certain roots of the secular equation are applied since the amplitudes of the assumed periodic response vanish. In the notation used below the second subscript denotes the root of the secular equation that is used in the calculation. For instance, A_{11} is the amplitude when the root V_1 is used. The amplitudes are

$$A_{11} \equiv 1 \qquad\qquad A_{12} = 0 \qquad A_{13} = \frac{\rho V_3^2 - C_{55}'}{C_{15}'}$$

$$A_{21} = 0 \qquad\qquad A_{22} \equiv 1 \qquad A_{23} = 0 \qquad\qquad (26)$$

$$A_{31} = \frac{\rho V_1^2 - C_{11}'}{C_{15}'} \qquad A_{32} = 0 \qquad A_{33} \equiv 1$$

The energy flow relationships for the modes of vibrational response in hexagonal materials are

For the root V_1 (Quasi-Longitudinal)

$$P_{x'} = C_{11}' A_{11}^2 + C_{55}' A_{31}^2 + 2C_{15}' A_{11} A_{31}$$

$$P_{y'} = 0 \qquad\qquad (27)$$

$$P_{z'} = C_{15}' A_{11}^2 + C_{35}' A_{31}^2 + (C_{55}' + C_{13}') A_{11} A_{31}$$

For the root V_2 (Pure Transverse)

$$P_{x'} = C_{66}' A_{22}^2$$

$$P_{y'} = 0 \qquad\qquad (28)$$

$$P_{z'} = C_{46}' A_{22}^2$$

For the root V_3 (Quasi-Transverse)

$$P_{x'} = C'_{11}A^2_{13} + C'_{55}A^2_{33} + 2C'_{15}A_{13}A_{33}$$

$$P_{y'} = 0 \qquad\qquad\qquad (29)$$

$$P_{z'} = C'_{15}A^2_{13} + C'_{35}A^2_{33} + (C'_{55} + C'_{13})A_{13}A_{33}$$

For this symmetry the above three equations (27, 28, and 29)
show that the y" component of the energy flow vector is
always zero. Thus the angle ψ defined on page 14 is always
zero and any deviation of the energy flow vector from the
propagation vector takes place in the x'-z' plane.

In order to demonstrate the validity of the perturbation
method solutions were computed on a Hewlett Packard 9810A
desk calculator and compared to published data for hexagonal
crystals, specifically zinc and beryl, as presented by M. J.
P. Musgrave.[4] Transformation equations using known values of
elastic constants were programmed and the velocities obtained
were in agreement to .05%. The energy flow components were
calculated and the angles of deviation from propagation
direction were consistent to within 2° of those presented by
Musgrave. The graphs on the following pages are examples of
results obtained for x-z plane propagation in hexagonal
crystals. In these graphs the deviation angle, δ, is plotted
as a function of the angle, θ, which the propagation vector
makes with the z-axis for each of the three modes. In addition

---

[4]M. J. P. Musgrave, "On the Propagation of Elastic Waves
in Aeolotropic Media," Proc. Roy. Soc. 226 (1954) p. 356.

the sign of all deviation angles in the cubic and hexagonal
cases has been reversed in order to compare the results with
Musgrave's data. Table I lists the known elastic constants
and densities required for the calculation.

TABLE I

	Elastic Constants $(10^{11}$ dynes/cm$^2)$					Density (gm/cm^3)
	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	
Zinc	14.3	1.7	3.3	5.0	4.0	7.1
Magnesium[5]	6.35	2.59	2.17	6.64	1.84	1.75

The metals Zinc and Magnesium are two different examples
of hexagonal material. The difference between C_{11} and C_{33}
in the two materials affects the response characteristics.
In both materials the Pure Transverse mode (T) has a non-zero
deviation angle for energy flow. This means that although
the mode is a pure vibration, associated with the root V_2 and
lying along the v' axis, the energy flow is non-zero and not
coincident with the x' axis (the propagation direction).

The response for Zinc indicates that no accidental mode
exists since the Quasi-Longitudinal (QL) response does not
become zero except at the end points $\theta = 0°$ (the c direction)
and $\theta = 90°$ (the x-y base plane). The absence of accidental

---

[5] W. P. Mason, ed., Physical Acoustics v. IIIB (New York,
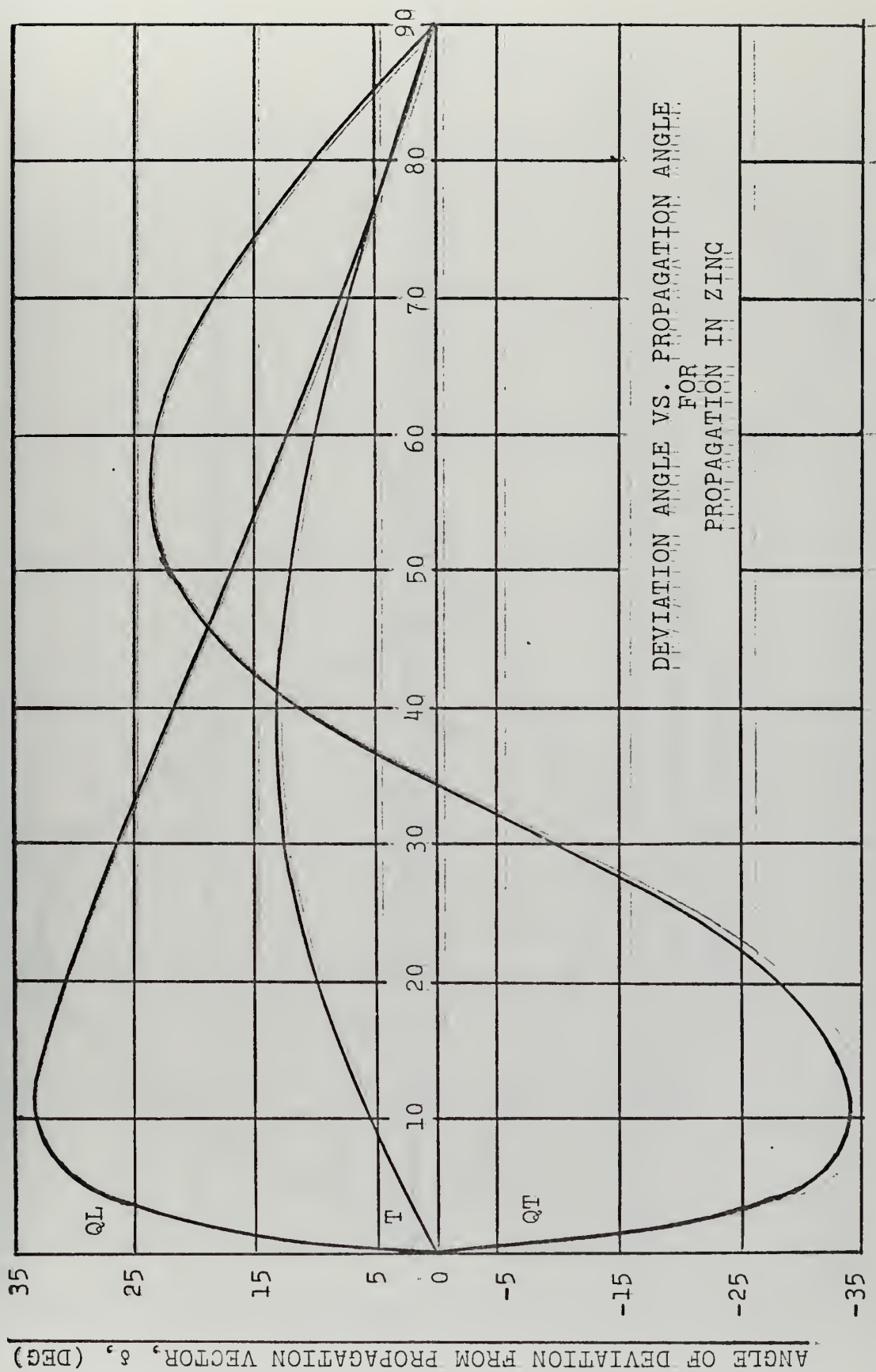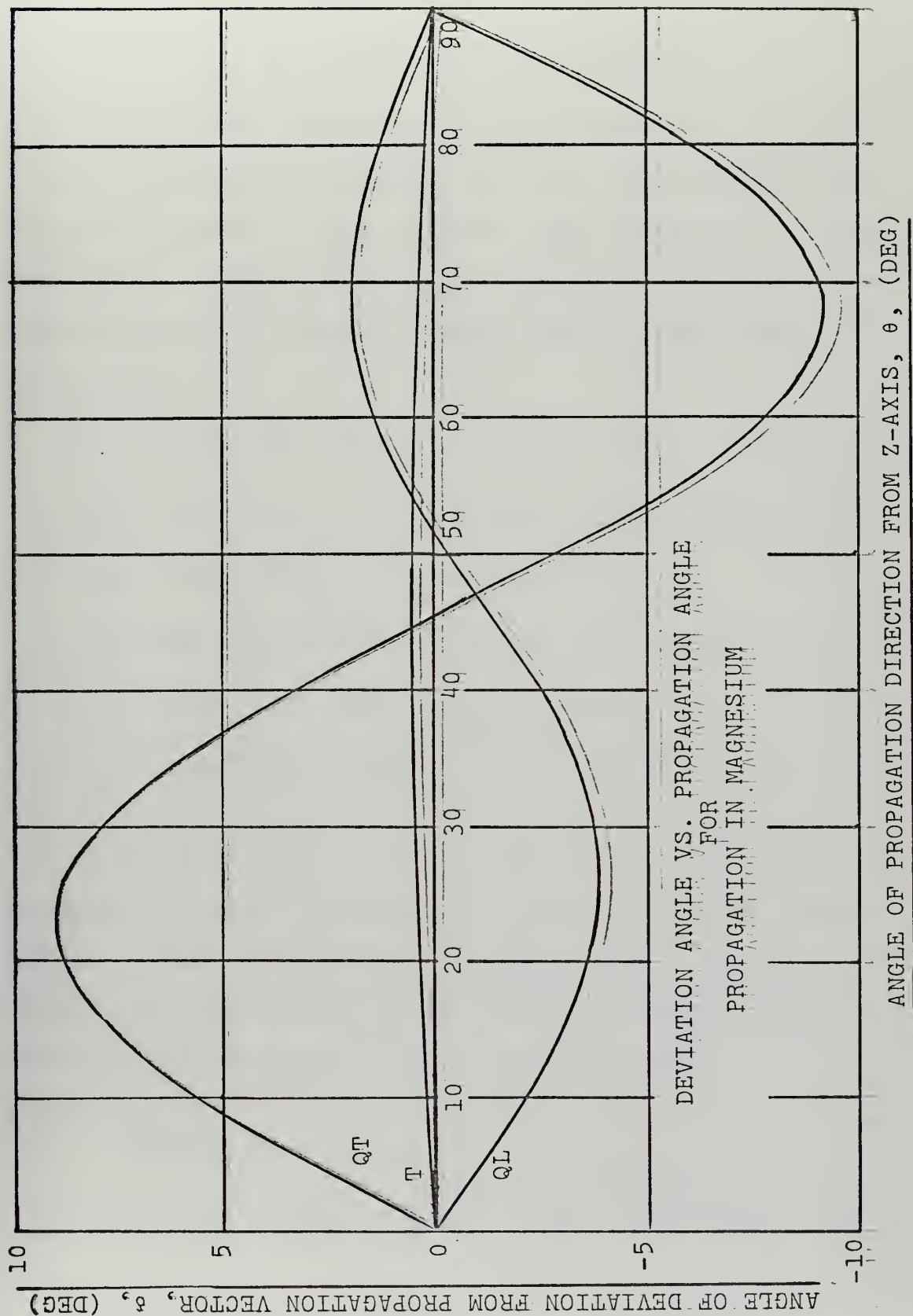1965), p. 32.

response can be verified by equation (23). The Quasi-
Transverse (QT) mode has a zero value between the end points
but this does not imply pure mode response since the amplitude
A_{13} has a non-zero value at this point. For Zinc the general
effect of elastic anisotropy on the energy flow is to channel
the energy of most of the waves toward the base plane.

An accidental pure mode is observable in Magnesium. The
Quasi-Longitudinal mode has a zero value at $\theta = 51.6°$.
Analysis of the amplitude shows that both A_{13} and A_{31} are
zero along this direction of propagation. Thus the amplitudes,
and hence the vibrational responses are colinear with the
primed coordinate system. The Quasi-Transverse mode has
essentially the same form of response as Zinc but is opposite-
ly directed. This is due to the difference in the value of
$(C_{11} - C_{33})$ for the two materials. The magnitude of the
deviation angles in Magnesium indicates that the material is
essentially isotropic.

DEVIATION ANGLE VS. PROPAGATION ANGLE
FOR
PROPAGATION IN ZINC

ANGLE OF PROPAGATION DIRECTION FROM Z-AXIS, θ, (DEG)

ANGLE OF DEVIATION FROM PROPAGATION VECTOR, δ, (DEG)

24

DEVIATION ANGLE VS. PROPAGATION ANGLE
FOR
PROPAGATION IN MAGNESIUM

25

VI. CUBIC SYMMETRY CRYSTALS

Calculations for cubic symmetry crystals follow the same pattern as that for hexagonal crystals. The conventional axes are parallel to the crystal basis vectors a, b, and c. The elastic constants are $C_{12} = C_{13}$, $C_{11} = C_{33}$, and $C_{66} = C_{44}$. Transformation of these constants leads to the equations shown below.

$$
C'_{11} = (\ell^4 + m^4 + n^4)C_{11} + 2(\ell^2 m^2 + \ell^2 n^2 + m^2 n^2)(C_{12} + 2C_{44})
$$

$$
C'_{55} = 2n^2 \alpha^{-2}(\ell^4 + m^4 + \ell^2 m^2)(C_{11} - C_{12} - 2C_{44}) + C_{44}
$$

$$
C'_{66} = 2\ell^2 m^2 \alpha^{-2}(C_{11} - C_{12} - 2C_{44}) + C_{44}
$$

$$
C'_{15} = -n\alpha^{-1}(\ell^4 + m^4 - n^2 \alpha^2)(C_{11} - C_{12} - 2C_{44})
$$

$$
C'_{16} = -\ell m \alpha^{-1}(\ell^2 - m^2)(C_{11} - C_{12} - 2C_{44})
$$

$$
C'_{56} = \ell m n \alpha^{-2}(\ell^2 - m^2)(C_{11} - C_{12} - 2C_{44})
$$

$$(30)$$

For propagation in the x-y, x-z, y-z or (110) planes the constants C'_{16} and C'_{56} vanish yielding a partially diagonal secular equation as for the hexagonal case. The velocity calculations are identical to those for hexagonal materials. The relations from the secular equations are

$$
V_2^2 = C'_{66}/\rho
$$

$$
V_{1,3}^2 = \frac{1}{2\rho}\left((C'_{11} + C'_{55}) \pm \sqrt{(C'_{11} + C'_{55})^2 - 4(C'_{11}C'_{55} - C'^2_{15})}\right)
$$

$$(31)$$

Further response analysis in the above planes yields amplitudes that vanish for certain modes of propagation and

elastic constants that vanish by choice of plane of propagation. Thus only C'_{46}, C'_{35} and C'_{13} remain to be inserted in the resultant energy flow equations which are similar to Eq. (25) for hexagonal symmetry. The graphs on the following pages show solutions for Aluminum with sound velocity propagation in the (100) plane (x-y plane) and the (110) plane ($\phi = 45°$). The results agree with Musgrave's data. The elastic constants for Aluminum are

$$C_{11} = 9.5 \times 10^{11} \text{ dynes/cm}^2$$

$$C_{12} = 4.9 \times 10^{11} \text{ dynes/cm}^2$$

$$C_{44} = 2.8 \times 10^{11} \text{ dynes/cm}^2$$

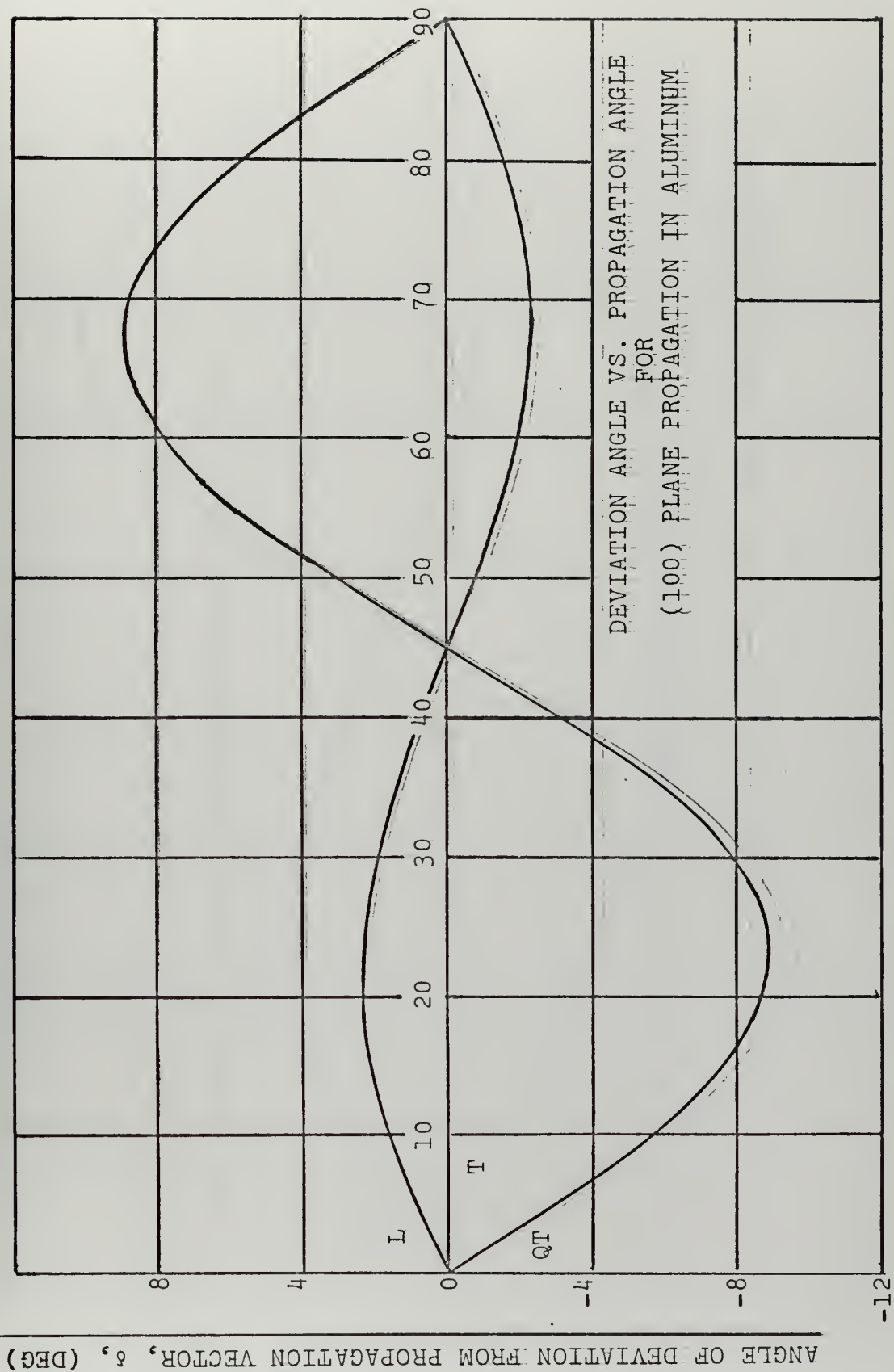The value for density is 2.65 gm/cm^3. These values are taken from Musgrave.

The results for (100) plane propagation in Aluminum show the existence of the accidental mode at $\theta = 45°$ which is predicted by Borgnis. The high symmetry of the response curves is expected in the case of cubic crystals. In addition the deviation angle for the Pure Transverse mode is zero. Thus the energy flow is colinear with the propagation direction. For propagation in the (110) and (100) planes the angle, ψ, is zero.

The response for (110) propagation merits particular attention. The Quasi-Longitudinal mode deviation angle goes to zero at $\theta = 54.6°$ which is the [111] direction. This is not an accidental mode but is indicative of the fact that C'_{15} is zero because of propagation direction. Thus the
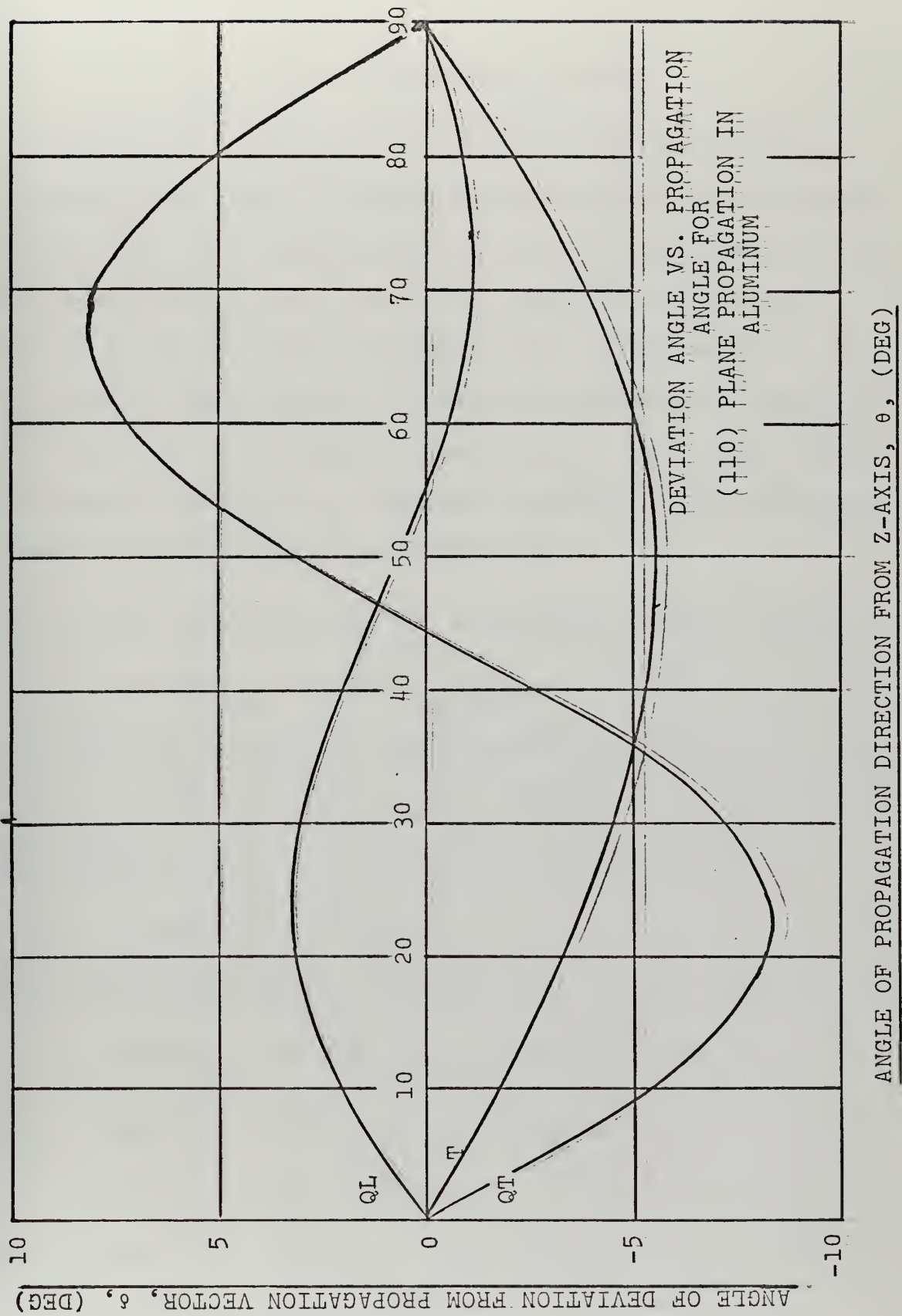
secular equation is diagonal and the three modes are pure.
In addition the velocities V_2 and V_3 are equal and the devi-
ation angles for these roots are equal and non-zero. The
phenomenon of internal conical refraction exists for this
propagation direction. It can be shown that $P_{x'}$ and
$(p_{y'}^2 + P_{z''}^2)^{1/2}$ are constant. Since the response for A_3 is
equal and opposite to that for A_2, the response for any
linear combination of the two, (making an angle γ, with the
y'-axis) would occur at twice the angle γ, in the $-\gamma$ direction.
In other words the energy flow describes a cone about the
propagation direction. If the amplitude for one mode is
rotated the response rotates in the opposite direction at
twice the angular frequency of rotation.

DEVIATION ANGLE VS. PROPAGATION ANGLE
FOR
(100) PLANE PROPAGATION IN ALUMINUM

ANGLE OF PROPAGATION DIRECTION FROM Z-AXIS, θ, (DEG)

ANGLE OF DEVIATION FROM PROPAGATION VECTOR, δ, (DEG)

DEVIATION ANGLE VS. PROPAGATION
ANGLE FOR
(110) PLANE PROPAGATION IN
ALUMINUM

ANGLE OF PROPAGATION DIRECTION FROM Z-AXIS, θ, (DEG)

ANGLE OF DEVIATION FROM PROPAGATION VECTOR, δ, (DEG)

30

VII. TETRAGONAL SYMMETRY

Solutions for tetragonal crystals represent a step forward since there is little data available to be compared with. The I.R.E. conventions define the z-axis parallel to the basis vector c and the x-axis parallel to the basis vector a, or the twofold symmetry axis. The two types of tetragonal class materials are distinguishable by the fact that $C_{16} = 0$ for Tetragonal I materials. The transformation of elastic constants is otherwise identical. The transformations for Tetragonal II materials are

$$C'_{11} = (\ell^4 + m^4)C_{11} + 2\ell^2 m^2 C_{12} + 2n^2 \alpha^2 (C_{13} + 2C_{44}) + n^4 C_{33}$$
$$+ 4\ell^2 m^2 C_{66} + 4\ell m(\ell^2 - m^2)C_{16}$$

$$C'_{55} = n^2 \alpha^{-2}(\ell^4 + m^4)C_{11} + 2\ell^2 m^2 n^2 \alpha^{-2}(C_{12} + 2C_{66})$$
$$- n^2 \alpha^2 (2C_{13} - C_{33}) + (1 - 2n^2)^2 C_{44} + 4mn^2 \alpha^{-2}(\ell^2 - m^2)C_{16}$$

$$C'_{66} = 2\ell^2 m^2 \alpha^{-2}(C_{11} - C_{12}) + n^2 C_{44} + \alpha^{-2}(\ell^2 - m^2)^2 C_{66}$$
$$- 4\ell m \alpha^{-2}(\ell^2 - m^2)C_{16} \tag{32}$$

$$C'_{15} = -n\alpha^{-1}(\ell^4 + m^4)C_{11} - 2\ell^2 m^2 n^{-1}C_{12} + n\alpha(1 - 2n^2)(C_{13} + 2C_{44})$$
$$+ n^3 \alpha C_{33} - 4\ell^2 m^2 n\alpha^{-1}C_{66} - 4\ell m n\alpha^{-1}(\ell^2 - m^2)C_{16}$$

$$C'_{16} = -\ell m \alpha^{-1}(\ell^2 - m^2)(C_{11} - C_{12} - 2C_{66})$$
$$+ \alpha^{-1}(\ell^4 + m^4 - 6\ell^2 m^2)C_{16}$$

$$C'_{56} = \ell m n \alpha^{-2}(\ell^2 - m^2)(C_{11} - C_{12} - 2C_{66})$$
$$- n\alpha^{-2}(\ell^4 + m^4 - 6\ell^2 m^2)C_{16}$$

Once again the choice of (100) or (110) plane propagation eliminates the constants C'_{56} and C'_{16} and the secular equation is partially diagonal. The energy flow calculations are simplified since C'_{14}, C'_{26}, C'_{36} and C'_{45} are identically zero. The remaining constants are

$$C'_{12} = (1-n^2)C_{12} + n^2 C_{13}$$

$$C'_{13} = n^2(1-n^2)(C_{11} + C_{33} - 4C_{44}) + (1-2n^2(1-n^2))C_{13}$$

$$C'_{25} = -n(1-n^2)^{1/2}(C_{13} - C_{12}) \tag{33}$$

$$C'_{35} = -n^3(1-n^2)^{1/2}C_{11} - n(1-n^2)^{1/2}(1-2n^2)C_{13}$$
$$\qquad + n(1-n^2)^{3/2}C_{33} - 2n(1-n^2)^{1/2}(1-2n^2)C_{44}$$

$$C'_{46} = n(1-n^2)^{1/2}(C_{44} - C_{66})$$

The resultant velocity and energy flow calculations are identical to those for hexagonal symmetry. The results are shown on the next graph for (100) plane propagation in Tin. The required data for calculation is given below.[6]

$$C_{11} = 8.27 \times 10^{11} \text{ dynes/cm}^2$$
$$C_{12} = 5.78 \qquad \text{"}$$
$$C_{13} = 3.42 \qquad \text{"}$$
$$C_{33} = 10.31 \qquad \text{"}$$
$$C_{44} = 2.69 \qquad \text{"}$$
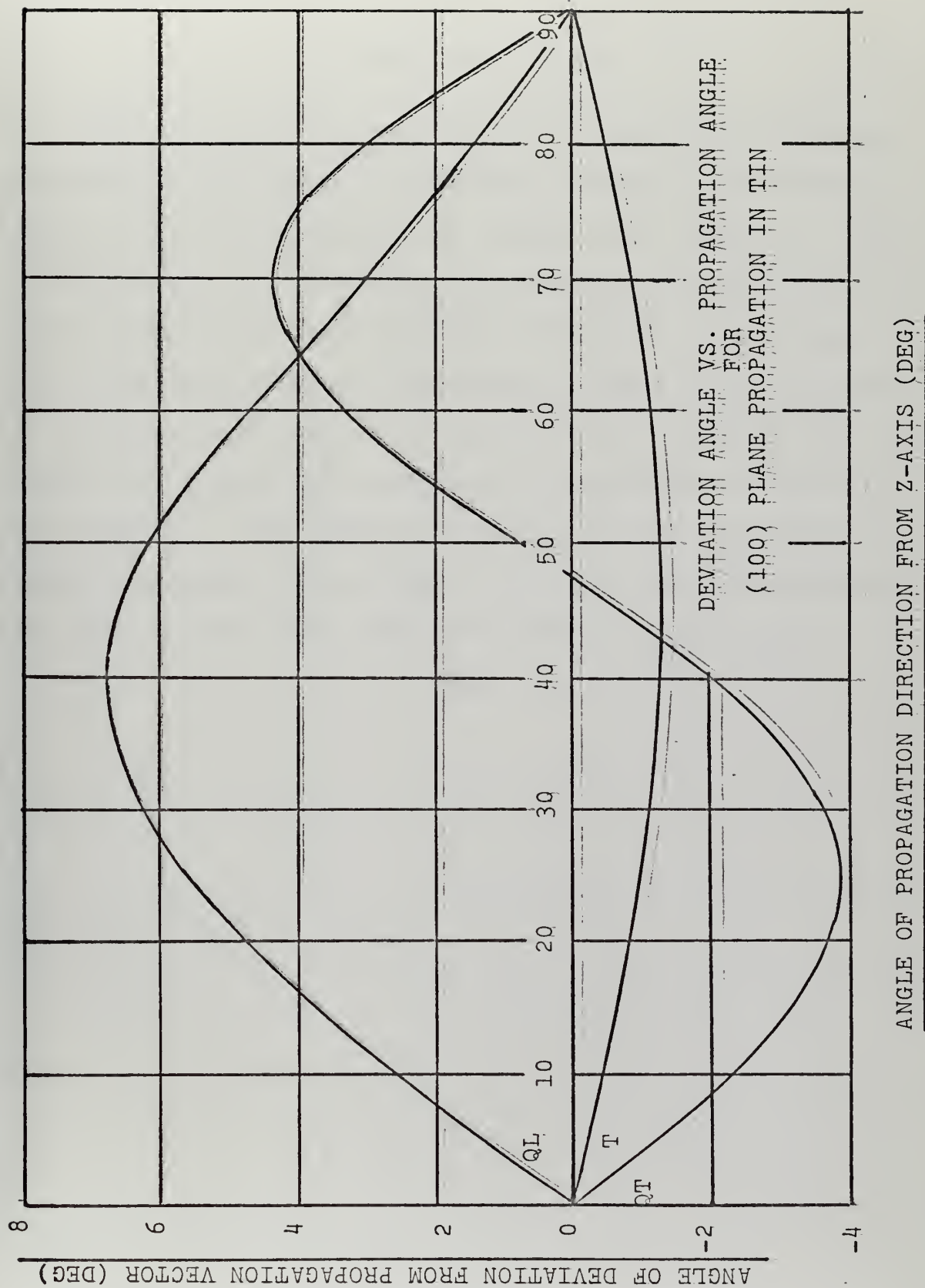$$C_{66} = 2.82 \qquad \text{"}$$
$$\rho = 7.39 \text{ gm/cm}^3$$

---

[6]Ibid.

The response is similar to that for Zinc in that no
accidental mode occurs. In addition the small deviation
angles again indicate that the material is essentially
isotropic. For the tetragonal results the deviation angles
are not reversed in sign.

DEVIATION ANGLE VS. PROPAGATION ANGLE
FOR
(100) PLANE PROPAGATION IN TIN

ANGLE OF PROPAGATION DIRECTION FROM Z-AXIS (DEG)

ANGLE OF DEVIATION FROM PROPAGATION VECTOR (DEG)

34

VIII. CONCLUSION

Agreement with published data indicates that the method
presented in this paper is a valid one and is particularly
useful in the determination of energy flow components. Thus
it is possible to calculate the direction of energy flow for
waves propagating in an arbitrary direction. The results
also show that, perhaps surprisingly, there may be directions
of propagation for which all the modes are pure but the trans-
verse wave energy flow vector and the propagation vector are
not colinear. This method can be extended to a crystal of
general symmetry. The effects of crystal stability and multi-
ple mode response are areas for further investigation.

LIST OF REFERENCES

1. Borgnis, F. E., "Specific Directions of Longitudinal Wave Propagation in Anisotropic Media," Phys. Rev. 98, (May 15, 1955), 1000-1005.

2. Cady, Walter G., Piezoelectricity v. I New York: Dover, 1946.

3. Farnell, G. W., "Elastic Waves in Trigonal Crystals," Canadian Journal of Physics, v. 39, (January, 1961), 65-79.

4. Love, A. E. H., A Treatise on the Mathematical Theory of Elasticity. New York: Dover, 1944.

5. Mason, Warren P., ed. Physical Acoustics. v. IIIB, New York: Academic Press, 1966.

6. Miller, G. F. and Musgrave, M. J. P., "Propagation of elastic waves in aeolotropic media. III," Proc. Roy. Soc. 236, (August 2, 1956), 352-284.

7. Musgrave, M. J. P., "Propagation of elastic waves in aelotropic media. I." Proc. Roy. Soc. 226, (November 23, 1954), 339-366.

8. Neighbours, J. R. and Schacher, G. E., "Determination of Elastic Constants from Sound Velocity Measurements in Crystals of General Symmetry," Journal of Applied Physics, 38 13 (December, 1967), 5366-5375.

9. Simmons, G. and Wang, H., Single Crystal Elastic Constants and Calculated Aggregate Properties. 2nd. ed. Cambridge: The M.I.T. Press, 1971.

10. Standard Committee, I.R.E., "Standard on Piezoelectric Crystals," Proc. I.R.E. 37 (December, 1949), 1378-95.

INITIAL DISTRIBUTION LIST

No. Copies

1. Defense Documentation Center
   Cameron Station
   Alexandria, Virginia   22314

2. Library, Code 0212
   Naval Postgraduate School
   Monterey, California   93940

3. Professor J. R. Neighbours, Code 61Nb
   Department of Physics
   Naval Postgraduate School
   Monterey, California   93940

4. LT Herbert C. Fauth, USN
   151 - 77 24th Road
   Whitestone, New York   11357

2

2

3

1

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author)	2a. REPORT SECURITY CLASSIFICATION
Naval Postgraduate School Monterey, California 93940	Unclassified
	2b. GROUP

3. REPORT TITLE

Acoustic Energy Flow in High Symmetry Crystals

4. DESCRIPTIVE NOTES *(Type of report and inclusive dates)*

Master's Thesis; June 1972

5. AUTHOR(S) *(First name, middle initial, last name)*

Herbert Carl Fauth

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
June 1972	39	10

8a. CONTRACT OR GRANT NO.	9a. ORIGINATOR'S REPORT NUMBER(S)
b. PROJECT NO.	
c.	9b. OTHER REPORT NO(S) *(Any other numbers that may be assigned this report)*
d.	

10. DISTRIBUTION STATEMENT

Approved for public release; distribution unlimited.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY
	Naval Postgraduate School Monterey, California 93940

13. ABSTRACT

The determination of elastic properties of crystals by sound velocity measurements is facilitated by use of a perturbation solution to the equations of motion for sound waves propagating in the crystals. Transformation equations can relate the solution for arbitrary propagation direction to an established crystal coordinate system. A method of calculating the acoustic components of the energy flow vector is developed for several high symmetry crystal classes. The validity of this method is herein confirmed and results are presented which are consistent with experimental data. A modern desk calculator was employed to determine solutions for hexagonal, cubic and tetragonal crystals.

DD FORM 1 NOV 65 **1473** (PAGE 1)

S/N 0101-807-6811

A-31408

KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	W-T	ROLE	WT	ROLE	WT
High Symmetry Crystals						